MATHEMATICAL MODELING OF RADIOLYSIS PROCESS OF WATER UNDER THE IMPACT OF LOW-ENERGY ELECTRONS

Y.D. Jafarov*

Institute of Radiation Problems, AZ1143, Baku, F.Aghayev 9

(Received April 29, 2011)

The radiolysis process of water (liquid phase) under the impact of low - energy electrons ($E = 1$, 2.5, 5, $10\,keV$) was mathematically modeled using Monte-Carlo, single collision and pacing methods on the base of Mathcad program. The radiation-chemical yields of the physical (single ionized molecular orbitals- $H_2O_j^+$ ($1a_1$, $2a_1$, $1b_2$, $3a_1$, $1b_1$), e_{sub}^- electron - lost its energy up to a primary electron - excited energy and electron-excited states: H_2O^* (A^1B_1, B^1A_1, Rydberg state, diffusion band, dissociative excitation and plasmon-H_2O^{**}) and physicochemical (OH, e_{aq}^-, H, H_3O^+, H_2, H_2O_2, O_2, OH^-, O_2^-, HO_2^-) phase products of the non-elastic collision of electrons and water molecules were determined.

PACS: 03.65.Pm, 03.65.Ge, 61.80.Mk

1. INTRODUCTION

Low-($0.05...10\,keV$), moderate-($10...100\,keV$) and high-energy ($100...5000\,keV$) electrons gradually lose their kinetic energies while passing through water in elastic and non-elastic collisions with water molecules. According to the mechanism of radiation energy loss at the physical phase of the non-elastic collision process ($< 10^{-15}\,sec.$) intermediate particles such as $H_2O_j^+$-direct single ionization of several molecular orbitals (MO), e_{sub}^- electron-lost its energy up to a primary electron-excited energy and electron-excited states: intermediate particles such as A^1B_1, B^1A_1 Rydberg state (Ry), diffusion band (ab), dissociative excitation (de) and plasmon (ce- collective excitation) are generating. As these particles have a strong effect on the physical, chemical, biological processes progressing in water and water solutions, it's possible to predict events which are likely to happen in the future by studying their roles in different fields of science (atomic, nuclear and plasma physics, astrophysics, modelling of atmospheric phenomena, radiochemistry, radiobiology etc.). Therefore, to theoretically and experimentally study the generation and consumption of these products is one of the main problems.

In the world literature the reliable values of the effective cross-section of a water molecule ionization under an electron impact (e^-, $2e^-$) was determined by authors [1-6] using different experimental methods and by authors [7-16] using different theoretical approaches.

There's no reference regarding water molecule excitation under an electron impact yet. Only authors [17-19] determined water electron-excitation states using a photoabsorption spectroscopy method. At the present time authors [20-24] have theoretically calculated the effective cross-section of water electron-excitation states using different polyempirical methods on the base of the experimental results.

The total effective cross-section of electron-water molecule scattering was identified by authors [25-30]. While comparing the results of the experimental and theoretical calculations it becomes evident that at the values of energy more than $30\,eV$ they coincide but at lower values some deviations are observed.

The radiation-chemical yields of the products generated at both phases (physical and physicochemical) of the water radiolysis process were theoretically calculated by authors [31-41] according to different approaches. There are some conformities with some errors between the theoretical and experimental results of different authors and our results.
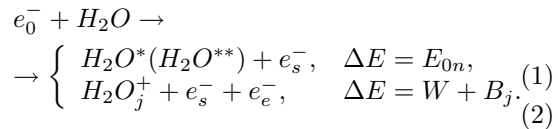
In the given work the radiolysis process of water (liquid phase) under the impact of low-energy ($T = 1.0$; 2.5; 5.0; $10\,keV$) electrons were mathematically modeled. The radiation - chemical yields of the primary products which were likely to generate in the physical ($< 10^{-15}\,sec.$) and physicochemical ($10^{-15}...10^{-12}\,sec.$) phases of the process were calculated. The more improved formula of Mott equation [7] was used to determine the effective cross - section of ionization process of molecular orbitals (MO), and the equations proposed by different authors were used to determine the effective cross - sections of electron - excited states of different types [13] in the model. Calculation was made on the base of Mathcad pro-

*Corresponding author E-mail address: azirp@rambler.ru

42

PROBLEMS OF ATOMIC SCIENCE AND TECHNOLOGY, 2011, N5.
Series: Nuclear Physics Investigations (56), p.42-47.

gram using Monte-Carlo, single collision and pacing methods.

2. THEORETICAL METHODS AND OBTAINED RESULTS

The energy balance between low-energy electrons and water molecules during a non-elastic collision can be simply expressed by $T = E_s + \triangle E$, here T and E_s are accordingly kinetic energies of an electron before and after collision, $\triangle E$ is the energy transferred to water molecule by an electron during collision. This energy is used for an electron-excitation of water molecule (1) and direct single ionization (2) of molecular orbitals (MO) ($1a_1, 2a_1, 1b_2, 3a_1, 1b_1$).

$$e_0^- + H_2O \rightarrow$$
$$\rightarrow \begin{cases} H_2O^*(H_2O^{**}) + e_s^-, & \triangle E = E_{0n}, \quad (1) \\ H_2O_j^+ + e_s^- + e_e^-, & \triangle E = W + B_j. \quad (2) \end{cases}$$

Here e_0^-, and e_e^- are accordingly incident, scattered and ejected electrons, $H_2O^+, H_2O^*, H_2O^{**}$ are correspondingly ionization, excitation and extreme excitation (plasmon) states. The transferred energy $\triangle E$ during these processes equals to an excitation energy of a molecule E_{on} in (1) case and the sum of the kinetic energy of an ejected electron W from j-molecular orbital and bound energy B_j of the correspondent orbital in (2) case. Kinetic energies of scattered and ejected electrons may accordingly change from $E_s = 0$ up to $E_s^{max} = T - B_j$ or from $W = 0$ up to $W^{max} = (T - B_j)/2$. A more improved formula [3] of Mott equation was used to calculate the effective cross - section of the single ionization of water molecule's $j - MO$:

$$\frac{d\sigma_j(W,T)}{dW} = \frac{S}{B_j(t + u + 1)} \left\{ \frac{1}{(w+1)^2} + \right.$$
$$\frac{1}{(w-1)^2} \frac{1}{(w+1)(t+w)} +$$
$$\left. \frac{4u}{3} \left[\frac{1}{(w+1)^3} + \frac{1}{(t-w)^3} \right] \right\}, \quad (3)$$

here, $t = \frac{T}{B_j}$, $w = \frac{W}{B_j}$, $u = \frac{U_j}{B_j}$, $S = 4\pi a_0^2 N_j \left(\frac{R}{B_j} \right)^2$, U_j and N_j are the kinetic energy and number of an electron correspondent to $j - MO$, a_0-Bohr radius, $R = 13.61\,eV$ is Rydberg energy. The values of B_j, N_j and U_j according to different molecular orbitals were given in Table 1. If we integrate the (3) expression for all possible values of ejected electrons' energies, i.e. from $W = 0$ up to W^{max}, we can get the expression describing the dependence of ionization effective cross - section on the kinetic energy of a primary (Fig.1) electron during non-inelastic collision corresponding to $j - MO$:

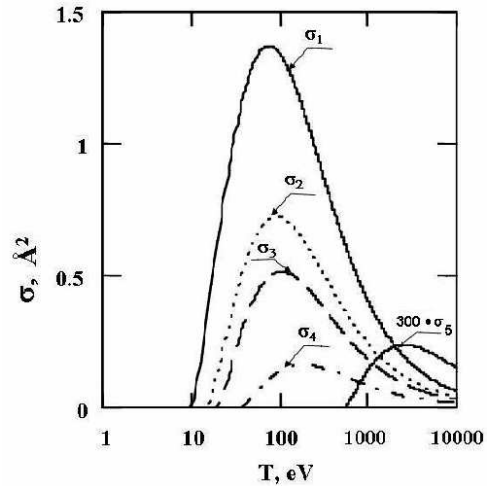$$\sigma_j(T) = \int_0^{W^{max}} \frac{d\sigma_j(W,T)}{dW} dW. \quad (4)$$

Fig.1. *Dependence of the effective cross - section of a direct single ionization corresponding to $j - MO$ ($\sigma_1 - 1a_1, \sigma_2 - 2a_1, \sigma_3 - 1b_2, \sigma_4 - 3a_1, \sigma_5 - 1b_1$) of water molecules under the impact of low - energy electrons*

In order to get the total effective cross - section of ionization (Fig.1) we should to sum the (4) expression according to the number of molecular orbitals (MO) [11]:

$$\sigma_{ion}(T) = \sum_{j=1}^{N_{MO}} \sigma_j(T). \quad (5)$$

Here $N_{MO} = 5$ is the number of molecular orbitals (MO) of a water molecule. During non-elastic collision between electrons and water molecules the effective cross-section of electron transformation from a ground state (0) to (n) excited state was calculated on the base of [13] expression:

$$\sigma_{0n}(T) = \frac{4\pi a_0^2 R}{T + B + E_{0n}} \left[a \ln \left(\frac{T}{R} \right) + b + c \frac{R}{T} \right]. \quad (6)$$

Here a, b and c are constants corresponding to $0 \rightarrow n$ junction and E_{0n} [13] is an excitation energy correspondent to that junction. Constants for each junction were chosen according to the values of radiation-chemical yield obtained from the experiments. The values of the constants and E_{0n} used in calculations were given in Table 2. In Fig.2 the dependence of the effective cross-sections of electron-excitation states ($\sigma_1 - A^1B_1, \sigma_1 - B^1A_1, \sigma_3$-Rydberg state ($Ry$), σ_4-diffusion band (db), σ_5-dissociative excitation (de) and σ_6-plasmon (ce)) in water under the impact of low-energy electrons on their energies were described.

In order to obtain the totally effective cross-section of electron excitation (Fig.1) (6) expression should be summed according to the number of excited states:

$$\sigma_{exc}(T) = \sum_n \sigma_{0n}(T). \quad (7)$$

Primary electrons or δ-electrons of a new generation formed by them lose part of their energy during each

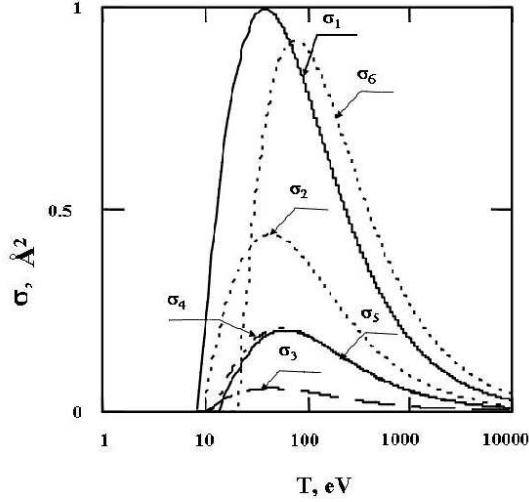non-elastic collision and this process continues till the next non-elastic collision of an electron energy.

Fig.2. *The dependence of the effective cross- sections of electron-excitation states ($\sigma_1 - A^1B_1, \sigma_1 - B^1A_1, \sigma_3$-Rydberg state (Ry), σ_4-diffusion band (db), σ_5-dissociative excitation (de) and σ_6-plasmon (ce)) in water under the impact of low-energy electrons on their energies*

The amount of the moderate energy $\Delta E(T)$ lost during each non-elastic collision of the electron with T energy with a water molecule was taken as an equivalent to the following expression [38, 39, 41]:

$$\Delta E(T) = \sum_n P_{0n}(T)E_n + \sum_j P_j(T)\varepsilon_j(T). \quad (8)$$

Here $P_{0n}(T) = \frac{\sigma_{0n}(T)}{\sigma_{tot}(T)}$ is the probability of transformation into n-excited state, $P_j(T) = \frac{\sigma_j(T)}{\sigma_{tot}(T)}$ is the probability of the event occurrence corresponding to the ionization of $j - MO$, $\sigma_{tot}(T) = \sum_n \sigma_{0n}(T) + \sum_j \sigma_j(T)$ - a total effective cross-section (Fig.3), $\varepsilon_j(T) = \int_{B_j}^{T} \varepsilon \frac{d\sigma_j(T)}{d\varepsilon}d\varepsilon$ - a moderate energy calculated for forming one electron-positive ion pair in $j - MO$ by the electron with T energy.
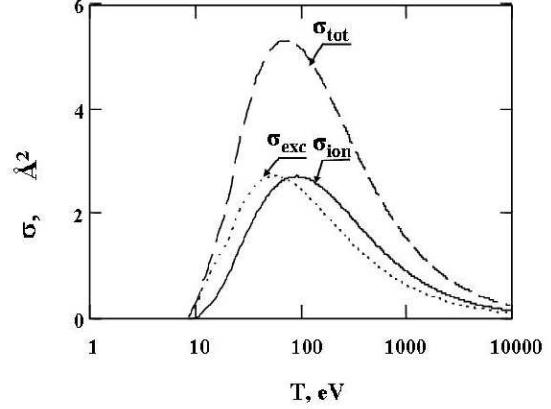

Fig.3. *The dependence of electron-excitation ($\sigma_{exc}(T) = \sum_n \sigma_{0n}(T)$), MO ionization ($\sigma_{ion}(T) = \sum_j \sigma_j(T)$) states in water under the impact of low-energy electrons and the full effective cross-section $\sigma_{tot}(T) = \sigma_{exc}(T) + \sigma_{ion}(T)$ on their energies*

Table 1. *The radiation-chemical yield of a direct single ionization corresponding to molecular orbitals (MO) of water molecule ($1a_1$, $2a_1$, $1b_2$, $3a_1$, $1b_1$) under the impact of low-energy electrons*

Molecular orbits	N	B_j, eV	U_j, eV	T, keV			
				1	2.5	5	10
$1a_1$	2	539.7	793.4	1.685	1.687	1.689	1.691
$2a_1$	2	36.88	70.71	0.951	0.950	0.954	0.957
$1b_2$	2	19.83	48.36	0.697	0.701	0.704	0.704
$3a_1$	2	15.57	59.52	0.259	0.260	0.263	0.265
$1b_1$	2	12.61	61.91	0.0003	0.0005	0.0007	0.0009

Table 2. *The radiation-chemical yields of electron-excited states (A^1B_1, B^1A_1, Rydberg states (Ry), diffusion band (db), dissosiative excitation (de) and plasmon (ce) states) formed in water under the impact of low-energy electrons*

Electron-excited state	Excitation energy, eV	Constants			T, keV			
		a	b	c	1	2.5	5	10
A^1B_1	8.4	0.7532	0.4751	-0.0675	0.870	0.877	0.872	0.875
B^1A_1	10.1	0.3900	0.1500	0.0015	0.412	0.407	0.413	0.409
Ry	12.26	0.0465	0.0282	-0.010	0.052	0.053	0.057	0.055
db	12.93	0.2380	0.0010	0.0265	0.267	0.269	0.264	0.260
de	14.1	0.2473	-0.010	0.0150	0.218	0.212	0.208	0.214
ce	21.4	1.2951	0.0120	-0.7532	1.089	1.086	1.087	1.094

On the base of the model calculations were made for the single ionization of five molecular orbitals (MO) and six electron-excited states of water molecules. The calculated values of the single ionization correspondent to $1a_1$, $2a_1$, $1b_2$, $3a_1$, $1b_1$ molecular orbitals (MO) were given in Table 1, and in Table 2 the calculated values of the radiation-chemical yields of A^1B_1, B^1A_1, Rydberg state (Ry), diffusion band (db), dissosiative excitation (de) and plasmon (ce) electron-excited states were given.

The products of the physical phase gradually (in the course of $10^{-15}...10^{-12}\,sec.$) lose their energies at the next physicochemical phase: at the result of e^-_{sub}-electrons' elastic collision and dipole relaxation and transform into thermal electrons and consequently solvates ($e^-_{sub} \rightarrow e^-_{aq}$), H_2O^+ ions transform into H_3O^+ ion and OH radical at the result of an ion-molecular reaction, and electron-excited molecules generate their next products due to relaxation, auto-ionization and dissociation. The next products [40] which were likely to be generated by the products of the physical phase in the course of $\sim 10^{-12}\,sec.$ were given in Table 3.

Table 3. *Percentage of the products which are likely to be generated by the products of the physical phase*

Products of the physical phase	$\dfrac{G}{100\,eV}$	Generation channels	Percentage, %
e^-_{sub}	3.592	e^-_{aq}	100
H_2O^+	3.592	$H_3O^+ + OH$	100
A^1B_1	0.870	$\begin{cases} H_2O \\ H_2 + OH \end{cases}$	$\begin{cases} 25 \\ 75 \end{cases}$
B^1A_1	0.412	$\begin{cases} H_2O \\ H_2 + H_2O_2 \end{cases}$	$\begin{cases} 45 \\ 55 \end{cases}$
$\begin{cases} R_y \\ db \\ de \end{cases}$	0.487	$\begin{cases} H_2O \\ H + OH \\ H_3O^+ + OH + e^-_{aq} \end{cases}$	$\begin{cases} 23 \\ 20 \\ 57 \end{cases}$
ce	1.089	$\begin{cases} H_3O^+ + OH \\ H^+ + OH \end{cases}$	$\begin{cases} 92.2 \\ 7.8 \end{cases}$

In the calculation carried out by us the radiation-chemical yields of the products generated in the physical and physicochemical phases of the radiolysis process progressing in the course of $\sim 10^{-12}\,sec.$ were determined and the obtained results (Table 4) were given in comparison with the theoretical [31, 42] and experimental ones [43,44] obtained by the authors.

Table 4. *Radiation-chemical yields of the products generated at the physicochemical phase ($10^{-15}...10^{-12}$ sec.) of the radiolysis process progressing in water under the impact of low-energy electrons*

Primary products	J.E.Turner [42]	I.Q.Kaplan [31]	Experimental results [43,44]	Our results
OH	8.4	5.85	5.9	5.624
e^-_{aq}	6.3	5.16	4.7	4.874
H	2.1	0.61	0.7	0.75
H_3O^+	6.3	5.16	4.8	4.874
H_2	0.3	0.39	0.45	0.227
H_2O_2	0.3	0.39	-	0.227
HO_2	-	-	-	-
O_2	-	-	-	-
OH^-	-	-	-	-
O_2^-	-	-	-	-
HO_2^-	-	-	-	-

The results obtained for the radiation-chemical yields of the active intermediate products generated in the physical and physicochemical phases of the radiolysis process progressing in water, calculated on the base of our model from the theoretical calculations and experiments conducted by different authors according to different approaches conform with some errors.

3. CONCLUSIONS

The processes progressing in water and water solutions under the impact of ionizing radiation (electron and ?-quantum) can be calculated on the base of this model. The model can be used to determine the processes progressing in aerosols of the atmosphere under the effect of space rays, changes in water and water solutions used in atomic and nuclear power-engineering as an energy-carrier or for different purposes, the nano-, micro and total absorption dose during radiating ancological patients by electrons and ?-quantum in the same and different directions as well as for the minimum selection of by-effects.

References

1. M.A. Bolorizadeh, M.E. Rudd // *Phys.Rev.A.* 1986, v.33, p.882.

2. K.W. Hollman, G.W. Kerby, M.E. Rudd, J.H. Miller, S.T. Manson //*Phys.Rev.A.* 1988, v.38, p.3299.

3. B.G. Lindsay and M.A. Mangan. *Photon and Electron Interactions with Atoms, Molecules and Ions.* "Landolt-Bornstein" v.I/17; Subvolume C, edited by Y. Itikawa. New York: "Springer", 2003.

4. H.C. Straub, B.G. Lindsay, K.A. Smith, and R.F. Stebbings // *J. Chem. Phys.* 1998, v.108, p.109.

5. M.V.S. Rao, I. Iga, and S.K. Srivastava // *J. Geophys. Res.* 1995, v.100, p.26421.

6. J. Schutten, F.J. de Heer, H.R. Moustafa, A.J.H. Boerboom, and J. Kistemaker // *J. Chem. Phys.* 1966, v.44, p.3924.

7. Y.K. Kim, M.E. Rudd // *Phys.Rev.A.* 1994, v.50, p.3954-3967.

8. M. Coplan, J.H. Moore, J.P. Doering // *Rev.Mod.Phys.* 1994, v.66, p.985.

9. Y.K. Kim, W. Hwang, N.M. Weinberger, M.A. Ali, M.E. Rudd // *J.Chem.Phys.* 1997, v.106(3), p.1026-1033.

10. M. Dingfelder, D. Hantke, M. Inokuti, H.G. Paretzke // *Radiat.Phys.Chem.* 1998, v.53, p.1-18.

11. Y.K. Kim, W.R. Johnson, M.E. Rudd // *Phys.Rev.A.* 2000, v.61, p.032702.

12. M.A. Haynes, B. Lohmann // *J.Phys.B.* 2000, v.33, p.4711.

13. Y.K. Kim, J.P. Desclaux // *Phys.Rev.A.* 2002, v.66, p.012708-12.

14. D. Emaietzoglou, K. Karava, G. Papamichael, M. Moscovich // *Phys. Med. Biol.* 2003, v.48, p.2355-2371.

15. W. Hwang, Y.K. Kim, and M.E. Rudd // *J. Chem. Phys.* 1996, v.104, p.2956.

16. C. Champion, J. Hanssen, and P.A. Hervieux // *J. Chem. Phys.* 2002, v.117, p.197.

17. W.F. Chan, G. Cooper, and C.E. Brion // *Chem. Phys.* 1993. v.178, p.387.

18. M. Gurtler, V. Saile, and E.E. Koch // *Chem. Phys. Lett.* 1977, v.51, p.386.

19. M. Chutjian, R.I. Hall, and S. Trajmar // *J. Chem. Phys.* 1975, v.63, p.892.

20. D. Gorfinkiel, L.A. Morgan, and J. Tennyson // *J. Phys.* 2002, B v.35, p.543.

21. W.A. Goddard and W.J. Hunt // *Chem.Phys.Lett.* 1974, v.24, p.464.

22. N.W. Winter, W.A. Goddard, and F. Bobrowicz // *J.Chem.Phys.* 1975, v.62, p.4325.

23. J.J. Olivero, R.W. Stagat, and A.E.S. Green // *J.Geophys.Res.* 1972, v.77, p.4797.

24. M. Zaider, D.J. Brenner, and W.E. Wilson // *Rad. Res.* 1983, v.95, p.231.

25. C. Szmytkowski // *Chem. Phys. Lett.* 1987, v.136 p.363.

26. A. Zecca, G. Karwasz, S. Oss, R. Grisenti, and R.S. Brusa // *J. Phys. B.* 1990, v.20, p.1500.

27. H. Nishimura and K. Yano // *J. Phys. Soc. Jpn.* 1988, v.57, p.1951.

28. Z. Saglam and N. Aktekin // *J. Phys.B.* 1990, v.23, p.1529.

29. Z. Saglam and N. Aktekin // *J. Phys. B.* 1991, v.24, p.3491.

30. M. Kimura, O. Sueoka, A. Hamada, and Y. Itikawa // *Adv. Chem. Phys.* 2000, v.111, p.537.

31. I.G. Kaolan, A.M. Miterev, V.Ya. Sukhanov // *KhVE*, 1986, v.20, N6, p.495-500.

32. M. Dingfelder, M. Inokuti, H.G. Paretzke // *Radiat.Phys.Chem.* 2000, v.59, p.255-275.

33. D. Emaietzoglou // *Radiat.Phys.Chem.* 2003, v.66. p.373-385.

34. C. Champion, J. Hanssen, P.A. Hervieux // *Phys.Rev.A.* 2001, v.63, p.052720-9.

35. C. Champion, J. Hanssen, P.A. Hervieux // *Phys.Rev.A.* 2002, v.65, p.022710-9.

36. D.S. Milne-Brownlie, S.J. Cavanagh, B. Lohmann, C. Champion, P.A. Hervieux, J. Hanssen // *Phys.Rev.A.* 2004, v.69, p.032701-4.

37. Y.K. Kim // *Phys.Rev.A.* 2001, v.64, p.032713-10.

38. A.A. Garibov, Ya.D. Jafarov, Ye.A. Shirshov, *4-th International Conference "Nuclear and Radiation Physics".* Almaata, 2003, p.335-337.

39. Ya.D. Jafarov, A.A. Garibov. // *International Conference "Physical-Chamical processes in Nonorganic Matherials"*, Kemerovo, Russia, 2004, v.1, p.32-34.

40. S. Uehara, H. Nikjoo // *J. Radiat. Res.* 2006, v.47, p.69-81.

41. Y.D. Jafarov, M.R. Hasanova, F.N. Nurmammadova // *The Fifth Eurazian Conference Nuclear Science and its Application*, Ankara, 2008, p.95-96.

42. J.E. Turner, R.N. Hamm, H.A. Wrighr, R,H. Rachie, J.L. Magee, A. Chatterjee, W.E. Bolch // *Radiat. Phys. Chem.* 1988, v.32, p.503-510.

43. A.K. Pikaev. *Modern Radiation Chemistry. Radiolysis of Gases and Liquids*, M: "Nauka", 1986, p.440.

44. V.L. Bugaenko, V.M. Byakov, V.L. Grishin // *Second Allunion Conference of Theoretical and Applied Radiation Chamistry*, Obninsk, Russia, 1990, p.29.

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА РАДИОЛИЗА ВОДЫ ПОД ДЕЙСТВИЕМ НИЗКОЭНЕРГЕТИЧЕСКИХ ЭЛЕКТРОНОВ

Я.Д. Джафаров

Проведено математическое моделирование радиолиза воды (жидкая фаза) под действием электронов с малой энергией ($E = 1, 2.5, 5, 10$ кэВ) при помощи программы Mathcad с использованием Монте-Карло, однократных столкновений и шагового методов. На основе этой модели вычислены радиационно-химические выходы следующих продуктов неупругих столкновений электронов с молекулами воды: физические (одноионизированные молекулярные орбитали - H_2O_j ($1a_1, 2a_1, 1b_2, 3a_1, 1b_1$) электроны с энергией, снизившейся до уровня с первым электронно-возбужденным состоянием - e^-_{sub}, и электронно-возбужденные состояния - H_2O^* (A^1B_1, B^1A_1, ридберговские состояния, полоса диффузии, диссоциативное возбуждение и плазмон - H_2O^{**}) и физико-химическая стадия ($OH, e_{aq}, H, H_3O^+, H_2, H_2O_2, HO_2, O_2, OH^-, O_2^-, HO_2^-$).

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ПРОЦЕСУ РАДІОЛІЗУ ВОДИ ПІД ДІЄЮ НИЗЬКОЕНЕРГЕТИЧНИХ ЕЛЕКТРОНІВ

Я.Д. Джафаров

Проведено математичне моделювання радіолізу води (фаза рідини) під дією електронів з малою енергією ($E = 1, 2.5, 5, 10$ кеВ) за допомогою програми Mathcad з використанням Монте-Карло, однократних зіткнень та шагового методів. На основі цієї моделі обраховані радіаційно-хімічні виходи слідуючих продуктів непружних зіткнень електронів з молекулами води: фізичні (одноіонізовані молекулярні орбіталі - H_2O_j ($1a_1, 2a_1, 1b_2, 3a_1, 1b_1$) електрони з енергією, пониженою до рівня з першим електронно-збудженим станом - e^-_{sub}, і електронно-збуджені стани - H_2O^* (A^1B_1, B^1A_1, рідберговські стани, полоса дифузії, дисоціативне збудження і плазмон - H_2O^{**}) і фізико-хімічна стадія ($OH, e_{aq}, H, H_3O^+, H_2, H_2O_2, HO_2, O_2, OH^-, O_2^-, HO_2^-$).